

Saddle scars: Existence and applications

R. Vilela Mendes

Grupo de Física-Matemática

Complexo II, Universidade de Lisboa

Av. Gama Pinto, 2, 1699 Lisboa Codex Portugal

e-mail: vilela@alf4.cii.fc.ul.pt

Abstract

A quantum scar is a wave function which displays an high intensity in the region of a classical unstable periodic orbit. Saddle scar are states related to the unstable harmonic motions along the stable manifold of a saddle point of the potential. Using a semiclassical method it is shown that, independently of the overall structure of the potential, the local dynamics of the saddle point is sufficient to insure the general existence of this type of scars and their factorized structure is obtained. Potentially useful situations are identified, where these states appear (directly or in disguise) and might be used for quantum control purposes.

1 Introduction

Until the early eighties it was widely believed that, for systems with an ergodic classical motion, the squared eigenfunctions must coincide, in the semiclassical limit, with the projection of the microcanonical phase space measure. This idea found solid ground on the mathematical results of Shnirelman[1], Zelditch[2] and Colin de Verdière[3]. On close scrutiny however, what these results state is that, for a quantum system that is classically ergodic, there is an eigenvalue sequence of density one such that the corresponding quantum densities $|\psi(x)|^2$ converge weakly to the Liouville measure. Therefore the observation of states that do not fit these expectations does not contradict

the mathematical results. For one thing the convergence may be very slow and, on the other hand, nothing forbids the existence of other subsequences converging to measures different from the Liouville measure.

In fact wave functions were found which are concentrated near the classical unstable periodic orbits. When this happens one says that *the quantum state is scarred by the unstable periodic orbit* or that one has a *quantum scar*. Such states have been observed at first in numerical simulations[4] [5] [6] and, more recently, experimental evidence was found[7] on a semiconductor quantum-well tunneling experiment.

The first theory of scars was proposed by Heller[5], other theoretical formulations followed, developed by several authors[8] [9] [10] [11]. Heller's theory studies the overlap integral

$$C(t) = \langle \Psi(t, x) | \Psi(0, x) \rangle \quad (1)$$

for a propagating wave packet which at time zero has a Gaussian shape and initial conditions (p_0, x_0) corresponding to an unstable periodic orbit. Expanding $\Psi(0, x)$ in energy eigenstates

$$\Psi(0, x) = \sum_n c_n \Psi_n(x) \quad (2)$$

one sees that the Fourier transform $S(E)$ of the overlap $C(t)$ is the spectral density weighted by the probabilities $|c_n|^2$.

$$S(E) = \sum_n |c_n|^2 \delta(E - E_n) \quad (3)$$

Now, if the period τ of the classical periodic orbit and the largest positive Lyapunov exponent λ are such that $e^{-\tau\lambda/2}$ is not very small, the overlap $C(t)$ will display peaks at times $n\tau$. As the wave packet spreads, the amplitude of the peaks decreases after each orbit traversal at the rate $e^{-\tau\lambda/2}$. The Fourier transform of $C(t)$ will therefore have peaks of width λ with spacing $\omega = \frac{2\pi}{\tau}$. Referring to (3) one concludes that only the eigenstates that lie under the peaks contribute to the expansion of the wave packet. Since the wave packet has an enhanced intensity along the region of the period orbit, this is expected to carry over to the contributing energy eigenstates. The stronger the overlap resurgences are, the stronger the effect is expected to be. Therefore the intensity of the effect varies like $1/\tau\lambda$.

The above qualitative derivation[5] of the scar effect is flawed if the product $\lambda d(E)$ (where $d(E)$ is the mean level density) is very large. Then the number of contributing eigenstates is very large and no individual eigenstate is required to show a significant intensity enhancement near the periodic orbit. Also the argument assumes the low period unstable orbits to be isolated. If there are several nearby orbits of different periods the argument breaks down. However, if it happens that many periodic orbits of the same period are present in the same configuration space region, the effect may even be enhanced. This is the situation for the periodic motions in the neighborhood of an unstable critical point (a saddle) of the potential $V(x)$. Near the critical point there are unstable harmonic periodic motions along the stable manifold of the critical point. As long as anharmonic corrections are unimportant, all the orbits will have the same period independently of their amplitude. The scars associated to these unstable periodic orbits are called *saddle scars* in this paper.

Whenever a dynamical system has a phase-space region with sensitive dependence to initial conditions, the periodic orbits in that region are unstable and, even when they are dense, they are a zero measure set in the smooth (Liouville) measure over the energy surface. Therefore, unstable classical orbits are in practice never observed, because all typical motions are aperiodic and uniformly cover the support of the Liouville measure. The phenomenon of quantum scars may therefore have far-reaching implications for the applications of quantum systems. Whenever an unstable periodic orbit scars a quantum eigenstate, the system may easily be made to behave like the unstable orbit by resonant excitation to the corresponding energy level. In this sense, scars are a gift of Nature, for they allow the exploration of dynamical configurations that in classical mechanics are washed away by ergodicity.

Saddle points are the typical critical points of generic (Morse) functions. Therefore, once their existence is established, saddle scars are expected to be quite abundant. In the remainder of the paper a semiclassical method is used to establish that, independently of the overall structure of the potential, the local dynamics of the saddle point is sufficient to insure the existence of this type of scars. Then, in the closing section, potentially useful situations are identified where these states appear (directly or in disguise) and may be used for quantum control purposes.

2 Semiclassical estimates

In the neighborhood of a saddle point, there is a choice of coordinates such that, up to higher order terms, the potential is

$$V(x) = \sum_i \sigma_i x_i^2 + \dots \quad (4)$$

For two dimensions $\sigma_1 > 0$ and $\sigma_2 < 0$. In this case one obtains the following result:

There are scar states concentrated along the stable manifold of the saddle point and, on the neighborhood of the stable manifold,

$$|\Psi_{\text{scar}}|^2 \propto \cos\left(\frac{W_n}{2\hbar}x_2^2\right) |\psi_n(x_1)|^2 \quad (5)$$

$\psi_n(x_1)$ being close to an harmonic oscillator wave-function and W_n a function of the monodromy matrix in the transverse direction. (Explicit expressions for W_n under different approximations are given below)

The result is obtained following Bogomolny's semiclassical construction of wave functions[8]. From the series expansion of the energy Green's function in terms of eigenfunctions it follows that the averaged squared wave function is proportional to the imaginary part of the Green's function

$$\langle |\Psi_{E_0}(x)|^2 \rangle \propto \langle \text{Im} G(x, x, E_0) \rangle \quad (6)$$

the average being taken over a small energy interval ΔE around E_0 , which corresponds, in the semiclassical approximation, to restrict the contributions to orbits with times of motion of order $\leq \frac{\hbar}{\Delta E}$. Likewise, if an average is taken over small intervals of the variable x , the dominant contributions come from classical trajectories for which the change of momentum on the closed orbit is small. I will discuss later the role of these two averages.

The next step is to use the semiclassical approximation for the Green's function

$$G(x_0, x, E) = \overline{G}(x_0, x, E) + \left(\frac{1}{\hbar}\right)^{(d+1)/2} G_{\text{osc}}(x_0, x, E) \quad (7)$$

$$G_{\text{osc}}(x_0, x, E) = i^{-1} \left(\frac{1}{2\pi i}\right)^{\frac{d-1}{2}} \sum_{\beta} \sqrt{|\det D_{\beta}|} \exp \left\{ \frac{i}{\hbar} S_{\beta}(x_0, x, E) - i \frac{\pi}{2} \nu_{\beta} \right\} \quad (8)$$

For the contributions in the neighborhood of a classical periodic orbit it is convenient to choose one of the coordinates along the orbit (x_1) and the others (x_i ; $i = 2, \dots, n$) along the transverse directions[12] [8]. On the neighborhood of an unstable periodic orbit along the stable manifold of the saddle point the action is expanded up to quadratic terms in the transversal coordinates and one has

$$G_{\text{osc}}(x, x, E) = \frac{1}{i(2\pi i)^{1/2}} \sum_{\beta} \frac{D^{1/2}(x_1)}{|\dot{x}_1|} \exp \left\{ \frac{i}{\hbar} \left(\bar{S}_{\beta} + \frac{1}{2} \sum_{i,j=2}^n W_{ij}(x_1) x_i x_j \right) - i \frac{\pi}{2} \nu_{\beta} \right\} \quad (9)$$

with $D(x_1)$ and $W_{ij}(x_1)$ functions of the monodromy matrix in the transverse coordinates

$$\begin{pmatrix} x_{\perp}(\tau_1) \\ p_{\perp}(\tau_1) \end{pmatrix} = \begin{pmatrix} m_{11}(x_1) & m_{12}(x_1) \\ m_{21}(x_1) & m_{22}(x_1) \end{pmatrix} \begin{pmatrix} x_{\perp}(0) \\ p_{\perp}(0) \end{pmatrix} \quad (10)$$

with

$$D(x_1) = |\det(m_{12}^{-1})| \quad (11)$$

$$W(x_1) = m_{12}^{-1} m_{11} + (m_{22} - 1) m_{12}^{-1} - (m_{12}^T)^{-1}$$

and τ_1 the period of the periodic orbit along x_1 . These expressions hold for any number of transverse directions. I now specialize to a two dimensional saddle point. Non-trivial orbits along the stable manifold are harmonic motions of period $\tau_1 = 2\pi\sqrt{\frac{m_1}{2\sigma_1}}$ independent of the amplitude of the oscillation. Therefore defining

$$D = \frac{\sqrt{2m_2\sigma_2}}{\sinh\left(2\pi\sqrt{\frac{m_1\sigma_2}{m_2\sigma_1}}\right)} \quad (12)$$

$$W = \frac{2 \cosh\left(2\pi\sqrt{\frac{m_1\sigma_2}{m_2\sigma_1}}\right) - 2}{\frac{1}{\sqrt{2m_2\sigma_2}} \sinh\left(2\pi\sqrt{\frac{m_1\sigma_2}{m_2\sigma_1}}\right)} \quad (13)$$

D and W do not depend on x_1 and the dependence on the transverse coordinate factors out for each term of the sum in Eq.(9). However, for each primitive trajectory, one also has to sum over multiple passings obtaining the following sum

$$\sum_n (2m_2\sigma_2)^{\frac{1}{4}} \sinh^{-\frac{1}{2}}(n\theta) \exp \left\{ \frac{i}{\hbar} \left(n\bar{S} + \frac{\cosh(n\theta) - 1}{2m_2\sigma_2 \sinh(n\theta)} x_2^2 \right) - i \frac{\pi}{2} n\nu \right\} \quad (14)$$

where $\theta = 2\pi\sqrt{\frac{m_1\sigma_2}{m_2\sigma_1}}$. There are two situations where simple closed form results may be obtained:

When $\exp(\theta) \gg 1$, the x_2 -dependence factors out from the sum and the result is

$$\langle |\Psi_E(x)|^2 \rangle \propto \left\langle \text{Im} \left\{ \exp \left(\frac{i}{\hbar} \frac{W}{2} x_2^2 \right) G(x_1, E) \right\} \right\rangle \quad (15)$$

$G(x_1, E)$ being the harmonic oscillator Green's function. From

$$G(x_1, E) = \sum_n |\Psi_n(x)|^2 \left\{ P \left(\frac{1}{E - E_n} \right) - i\pi \delta(E - E_n) \right\} \quad (16)$$

it follows that the principal part drops out under averages over small energy intervals and the result (5) follows with $W_n = W$ for $n = 1, 2, \dots$. The lowest lying state however corresponds to the orbit of the unstable fixed point and the period of this orbit is no longer τ_1 . The value of W_0 in this case may be calculated by considering an orbit from the coordinate $(0, x_2)$ to the fixed point $(0, 0)$ and back along the unstable manifold, which is equivalent to take the limit $\sigma_1 \rightarrow 0$ in Eq.(13). Then

$$W_0 = 2\sqrt{2m_2\sigma_2} \quad (17)$$

If $\exp(\theta)$ is not large then the x_2 -dependence does not factor out in the sum (14). Notice however that the sum in (14) is not a sum over multiple passings of the same orbit, but a sum over different orbits because, for $x_2 \neq 0$, the initial and final momentum are different, and the difference grows with n . Therefore if, in addition to the average over small energy intervals, one also averages over small coordinate intervals then, the contribution of the primitive orbit dominates the leading semiclassical approximation. The same factorization of the x_2 -dependence, as before, is obtained. However, the $\psi(x_1)$ function in this case is not exactly an harmonic oscillator wave functions, but a function corresponding to a sum restricted to the primitive orbits.

3 Applications

The canonical form of the potential near a saddle point establishes a local separation of variables which, of course, does not hold far away from the saddle point. However, what the semiclassical estimate of the previous section

shows is that the local dynamics of the saddle point is sufficient to insure the local existence of a factorized quantum state (5). If the separation of variables extends over a sufficiently large range then, the transverse shape of the wave function may be approximated by the solution of a one dimensional problem. Consider, for example a one-dimensional Hamiltonian

$$H = -\frac{1}{2m} \frac{d^2}{dx^2} + 2g \cos(x) \quad (18)$$

with 2π -periodic boundary conditions. The eigenstates are Mathieu functions and there is a state of energy slightly above $2g$ with the squared amplitude $|F|^2$ as shown in Fig.1 (for $g = 50$, $\frac{1}{2m} = 1$, $E = 101.189$). In the figure the state is also compared with the local approximation following from (5) and (17). The width of the state depends on the factor $\sqrt{2mg}$ and the energy is approximately $2g$ plus the kinetic localization energy. For an higher dimensional problem one must also add the quantized energy of the harmonic oscillation along the stable manifold. These considerations provide a simple rule for the approximate energies at which saddle scars are expected to be found.

Among the physical situations where saddle scars might appear, an interesting example is probably the quantum collision of systems containing both attractive and repulsive interactions (chemical ions, nuclei, etc)[13]. When a system contains several positive and negatively charged particles, there are classical configurations of close proximity of the particles which are of low energy because the repulsion between the like-charged particles is compensated by the attraction of unlike-charged particles. These configurations however are highly unstable and the chance to observe (or stabilize) them in classical mechanics is nil. They are zero measure configurations in the energy surface. For smooth potentials these unstable configurations would be saddle points of the potential, hence they are expected to give rise to saddle scars. These states would correspond to well defined energy levels and might be prepared by resonant excitation. That is, quantum control through scars makes accessible some states that, classically, are essentially unobservable.

Another interesting aspect of saddle scars is their generality, because saddle points are the typical critical points of generic functions. There are also other features of the classical phase space which the wave functions imitate and that, in some limit or by change of coordinates, may be related to the saddle scars. This concerns in particular the regularization of singular

potentials. An example is the collision states found for a three-dimensional periodic Coulomb problem[13]. In this case the quantum collision states correspond to wave functions concentrated along a phase space feature which is not an actual orbit, but the separatrix of two classes of unstable orbits.

In Jacobi coordinates ($r = x_1 - x_2$, $\eta = x_3 - \frac{1}{2}(x_1 + x_2)$) the potential between three unlike-charged particles is

$$V(r, \eta) = \frac{1}{|r|} - \frac{1}{\left|\frac{r}{2} - \eta\right|} - \frac{1}{\left|\frac{r}{2} + \eta\right|} \quad (19)$$

The dynamics of binary collisions in the three-body problem may be regularized, but the case of interest here is a triple collision which, except for exceptional cases[14], is not regularizable. The potential, however, may be regularized by addition of a small quantity to the definition of the distances

$$|\rho|_\epsilon = \left(\rho_1^2 + \rho_2^2 + \rho_3^2 + \epsilon^2\right)^{\frac{1}{2}} \quad (20)$$

In the neighborhood of the triple collision point $\vec{r} = \vec{\eta} = 0$, the regularized potential is

$$V_\epsilon = -\frac{1}{\epsilon} - \frac{1}{4\epsilon^3} |r|^2 + \frac{1}{\epsilon^3} |\eta|^2 + \dots \quad (21)$$

and this is a saddle point with three stable and three unstable directions. According to the discussion above one would expect the quantum collision states to have scarred wave functions concentrated along the stable manifolds and with a small dispersion in the transverse (unstable manifold) directions. This is the situation that is indeed found in the numerical computations[13] of the three-dimensional periodic Coulomb problem. It shows that the effect seems to survive the $\epsilon \rightarrow 0$ limit. Triple collisions in a 3-dimensional 3-body problem lie on an analytic 10-dimensional submanifold of the 12-dimensional dynamical manifold. Hence it is a zero measure effect, essentially non-observable in classical systems. It is interesting that, through the scar effect, they do correspond to well-defined energy levels, accessible by resonant excitation.

4 Figure caption

Fig.1 - One dimensional density for a wave function concentrated around an unstable point and the semiclassical approximation (+).

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Fig. 1

